Sandia National Laboratories

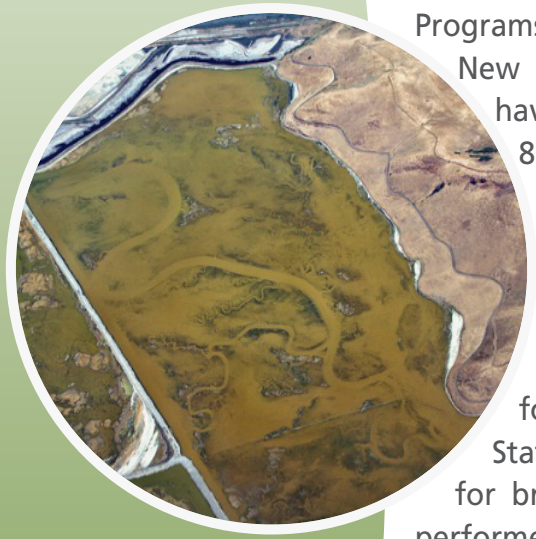
Energy, Climate, & Infrastructure Security

Computer Modeling of Chemical and Geochemical Processes in High Ionic Strength Solutions

Computer modeling of chemical and geochemical processes in high ionic strength solutions is a unique capability.

Description

Computer modeling of chemical and geochemical processes in high ionic strength solutions is a unique capability within Sandia's Defense Waste Managment Programs located in Carlsbad, New Mexico. We currently have use of EQ3/6 Version 8a, a version of EQ3/6 that is tailored specifically for high ionic strength systems in addition to a library of Pitzer parameters for elements found in WIPP brines. State of the art calculations for brines at WIPP are being performed using EQ3/6 Version 8a for the fourth certification of the WIPP repository.



Aerial photograph of brine lake in Utah

The first certification of WIPP

For the first certification of WIPP, dissolved radionuclide concentrations were calculated for WIPP brines estimated to be between pH 8 and pH 11 once equilibrium is established with the MgO backfill material. Concentrations were calculated using FMT (Fracture Matrix Transport) Version 2.4 developed at SNL to incorporate Pitzer's equations for both forward and reverse modeling in solutions with high ionic strengths up to saturation of salts.

The second certification of WIPP (2004)

An expanded database of thermodynamic data and Pitzer data was obtained from the literature where possible, and developed through laboratory testing where literature data was not available. Using NONLIN Version 2.01 Pitzer data were derived. This data set was thoroughly reviewed to assure its quality and internal consistency. For comparison purposes, EQ3/6 calculations using a dated version of EQ3/6 were performed and compared to the FMT calculations. Inconsistencies were identified at that time.

The third certification of WIPP (2009)

The database of thermodynamic data and Pitzer data was expanded for elements in WIPP brines such as borate, iron, and lead. These parameters were developed through research performed within Sandia's Defense Waste Management Programs. Sandia's Defense Waste Management Programs has full laboratory capabilities to perform and analyze solubility experiments in brine

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and mineral systems. In addition, Sandia's Defense Waste Management Programs has extensive experience in usage of the computer code, EQBRM, with user's choice of activity coefficient model, to calculate speciation and solubility in hydrothermal processes to ultra-high temperatures and pressures of interest to model geochemical processes up to magmatic temperatures and pressures, as long as there are relevant supporting thermodynamic data at desired temperatures and pressures. For the third certification of the WIPP, contaminant concentrations in brine were calculated using FMT.

The fourth certification of WIPP (2014)

For the fourth certification of WIPP, contaminant concentrations in brine are being calculated using EQ3/6 Version 8a which has been fully qualified for use in WIPP calculations. This version of the code was modified by researchers within Sandia's Defense Waste Management Programs to remedy errors overcome by limitations found in previous versions that limited the usefulness of those versions to high ionic strength brines. This specialized version of EQ3/6 can accommodate WIPP brines.

Publications

Experimental Determination of Solubilities of Sodium Tetraborate (Borax) in NaCl Solutions, and A Thermodynamic Model for the Na-B(OH)3-Cl-SO4 System to High Ionic Strengths at 25°C. 2012. Sandia National Laboratories, Albuquerque, NM. SAND2012-9674J.

Iron and Lead Corrosion and Solubilities in Brines. 2009. Sandia National Laboratories, Albuquerque, NM. SAND2009-5831P.

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